

# Accepted Manuscript

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PII: S0022-5096(16)30764-5  
DOI: [10.1016/j.jmps.2017.03.016](https://doi.org/10.1016/j.jmps.2017.03.016)  
Reference: MPS 3086



To appear in: *Journal of the Mechanics and Physics of Solids*

Received date: 21 October 2016  
Revised date: 20 February 2017  
Accepted date: 26 March 2017

Please cite this article as: Karol Kulasinski , Dominique Derome , Jan Carmeliet , Impact of Hydration on the Micromechanical Properties of the Polymer Composite Structure of Wood Investigated with Atomistic Simulations , *Journal of the Mechanics and Physics of Solids* (2017), doi: [10.1016/j.jmps.2017.03.016](https://doi.org/10.1016/j.jmps.2017.03.016)

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# Impact of Hydration on the Micromechanical Properties of the Polymer Composite Structure of Wood Investigated with Atomistic Simulations

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## Abstract

A model of the secondary layer of wood cell wall consisting of crystalline cellulose, hemicellulose, and lignin is constructed and investigated with molecular dynamics simulations in the full range of hydration: from dry to saturated state. The model is considered a composite with the cellulose fibrils embedded in hemicellulose and lignin, forming a soft amorphous matrix. Its complex structure leads to nonlinear and anisotropic swelling and mechanical weakening. The water diffusivity through the pores is affected by an interplay between stiff cellulose fibers and weakening amorphous polymers. The formation and breaking of hydrogen bonds within the polymers and at the interfaces is found to be the underlying mechanism of adsorption-induced mechanical softening. The model is tested for adsorption isotherm, mechanical moduli, hydrogen bonds, and water diffusivity that all undergo a substantial change as the hydration increases. The determined physical and mechanical properties, changing with hydration, agree qualitatively with experimental measurements.

**Keywords:** hydration; porosity; swelling; weakening; hydrogen bonds; diffusion.

## Introduction

The extraordinary mechanical properties of wood tissue, such as high stiffness-to-density ratio, anisotropy, or non-linearity, are the result of both wood hierarchical organization and the composite structure of wood cell wall<sup>1-3</sup>. Wood tissue (xylem) is composed of tubular cells with various void sizes and arrangements: tracheid for softwood and vessel and fiber for hardwood, that are responsible for a broad range of physical and mechanical properties of wood. At the microscopic scale, the wood cell wall is composed of different layers with varying: thickness, structural arrangement, and chemical composition<sup>1,4-7</sup>. Among the layers, the largest by mass and volume is the secondary layer S2, accounting for 80% of a tracheid cell volume<sup>8</sup>. The high stiffness of S2 layer, approximately 80 GPa in longitudinal direction, is the result of the parallel-stacking of the cellulose microfibrils<sup>9</sup>. The microfibrils form a composite structure together with the hemicellulose and lignin polymers playing the role of soft amorphous matrix<sup>10-13</sup>. Wood is a strong water absorber and its properties change drastically as its water content increases<sup>1,4,14-20</sup>. During adsorption, the wood cell wall undergoes an important decrease of elastic moduli accompanied by swelling<sup>19,20</sup> and an increase in diffusion coefficient of the adsorbed water<sup>21</sup>. The water-absorbing wood polymers, hemicelluloses and lignin, alone display a similar, water-sensitive, behavior<sup>4,22,23</sup>. Despite numerous experimental and numerical studies, the mechanisms of coupling mechanical and adsorption effects in wood cell wall are not yet fully understood. This includes molecular-level mechanism of how does adsorption at interfaces impact the overall mechanical properties, why do the weakening curves display an exponential-like shape, and how does the role of crystalline cellulose influence the swelling of other S2 constituents?

The hydroxyl groups of cellulose and hemicellulose are the sorption sites for water molecules responsible for hydrophilicity of wood cell wall<sup>24-26</sup>. There is an evidence that an appreciable fraction of the total sorption is associated with sorption at the surfaces of crystallites<sup>27,28</sup>. Taking into account the dimensions of a cellulose microfibril in wood, a considerable amount of crystalline chains can be on the surface and thus accessible to water because of the disordered OH groups that are accessible to water molecules and are hydrogen-bonded

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